

2-amino-3-(4-chlorophenyl)sulfonylpropanoic acid
5445-04-5 | DTXSID30396827

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 155 °C

Global applicability domain: Inside

Local applicability domain index: 3.88e-01

Confidence level: 6.22e-01

Nearest Neighbors from the Training Set

Image not found

4-(2-Hydroxyethanesulfonyl)benzene-1-sulfonamide

Measured: 165

Predicted: 156

Image not found

4-(3-Hydroxypropane-1-sulfonyl)benzene-1-sulfonamide

Measured: 150

Predicted: 149

Image not found

3-Fluoro-4-(3-hydroxypropane-1-sulfonyl)benzene-1-sulfonamide

Measured: 130

Predicted: 141